Truncated Determinant Approach to Light Dynamical Quarks

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Virtual quark effects in lattice QCD are studied in an approach where the infrared modes are included in a precise and gauge-invariant manner. At fixed physical volume the required number of modes does not increase in the continuum limit, and the acceptance is tolerable even for very light quark masses. Topological charge distributions at varying quark mass, and the static quark potential, showing the onset of string-breaking, are presented in both QED2 and QCD4.

1. Role of Infrared Dirac Modes in Non-perturbative Lattice QCD

It is well known that the quenched approximation seriously mutilates the infrared Dirac structure of lattice QCD. Among the many undesirable effects of this truncation of the theory one finds
(1) Nonintegrable quark propagator singulariities render the Wilson-Dirac quenched path integral *undefined* [1], a pathology which surfaces in explicit Monte Carlo simulations in the guise of "exceptional configurations" leading to uncontrolled statistical fluctuations.
(2) Quenched chiral logarithms complicate the extraction of reliable chiral extrapolations.
(3) Nontrivial topology (i.e. nonzero topological charge) is not suppressed in the light quark limit.
(4) Characteristic physical phenomena induced by virtual quark pairs- string-breaking, rho decay, etc- are absent.
Inclusion of the infrared quark modes, characterized as the low eigenvalues of the hermitian operator $H \equiv \gamma_5(\slashed{D}-m)$, allows a precise gauge invariant truncation [2] which interpolates in a natural way between the quenched and fully unquenched theory, eliminating all the aforesaid problems. The spectrum of H can be thought of as characterizing the gauge-invariant off-shellness of the quark field, as the eigenvalues are gauge-invariant and reduce in the free theory to $\pm\sqrt{p^2+m^2}$ for a quark mode of Euclidean momentum p. We

shall discuss simulations in which all modes up to a cutoff somewhat greater than (typically, about twice) Λ_{QCD} are included in the quark determinant part of the full Boltzmann weight. It turns out that accurate inclusion of the remaining ultraviolet modes [3] requires a cutoff at a fixed number of eigenvalues rather than in energy.

2. Implementing a Gauge Invariant Truncation of the Quark Determinant

The spectrum of the hermitian Dirac operator H consists of eigenvalues $\lambda_i(A)$ which are gauge-invariant functions of the gauge field A. For QCD4 the dimension of H is $\mathcal{N} = 12V$, with V the lattice volume, and it is convenient to order the spectrum with the index i running from $-\mathcal{N}/2$ to $\mathcal{N}/2$ with $\lambda_i < \lambda_{i+1}$. With the conventional lattice normalization the spectrum extends from $-(1+8\kappa)$ to $+(1+8\kappa)$ (roughly, from -2 to +2) with the physical branch extending up to $|\lambda| \simeq 0.5$. We shall describe the results of simulations in which the full quark determinant contribution is replaced by $\mathcal{D}_{N_\lambda}(A) \equiv \prod_{i=-N_\lambda}^{+N_\lambda} \lambda_i(A)$. For QCD4 we choose $N_\lambda \simeq 50$, corresponding to $\lambda_{N_\lambda} \simeq 370$ Mev, in other words, somewhat larger than the low energy scale Λ_{QCD}. Low eigenvalues are obtained by the following Lanczos scheme:
(1) Starting with a randomly chosen initial vector v_1, an orthonormal sequence $v_1, v_2, v_3, ..v_{N_L}$ is generated by the standard recursion:

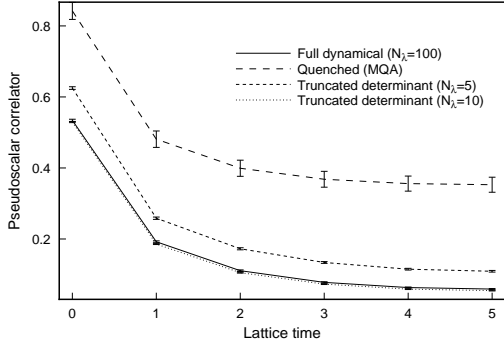Figure 1. Pseudoscalar correlators in QED2

Figure 2. Q_{top} histogram in QED2

$$v_{k+1} = \frac{1}{\beta_k} H v_k - \frac{\beta_{k-1}}{\beta_k} v_{k-1} - \frac{\alpha_k}{\beta_k} v_k$$

with the constants α_k, β_k determined from overlaps of generated vectors. In the basis of the v_i, H is tridiagonal. The corresponding real symmetric tridiagonal matrix T_{N_L} has the α_k on the diagonal and the β_k on the sub (and super) diagonal.

(2) A Cullum-Willoughby sieve [4] is applied to remove spurious eigenvalues.

(3) The remaining "good" eigenvalues converge most rapidly in the needed infrared portion of the spectrum. The stability and accuracy of the converged eigenvalues has been checked extensively by gauge transforming the gauge field.

(4) The diagonalization of the T_{N_L} matrix (typically, of order 10,000 in the QCD case) can be completely parallelized using the Sturm sequence property [5] of tridiagonal matrices which allows nonoverlapping parts of the spectrum to be independently extracted by a bisection procedure.

3. Truncated Determinant Simulations in QED2

We have tested the truncated determinant approach in two-dimensional abelian gauge theory (QED2) on 10x10 and 16x16 lattices at $\beta = 4.5$ and for bare quark masses $m_0 = 0.06$ and 0.10. Superrenormalizability implies that higher momentum modes are essentially inert (the product of the upper 90% of the spectrum is practically constant) and one finds complete agreement between exact dynamical simulations and those using only the $2N_\lambda = 20$ lowest eigenmodes
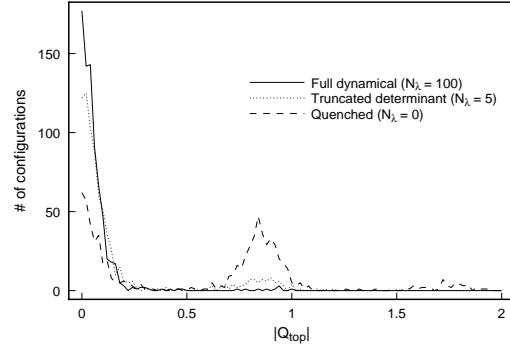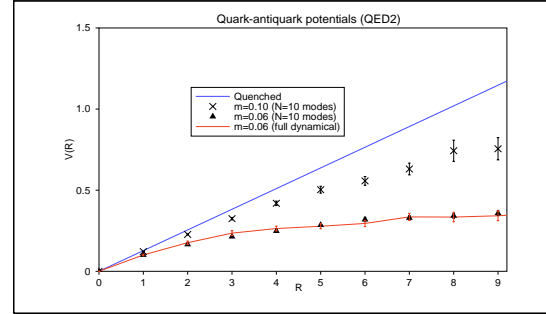

Figure 3. Quark-antiquark potentials in QED2

of the (hermitian) Wilson-Dirac operator. The simulation procedure used was as follows. A pure gauge update consisting of 5 metropolis sweeps was followed by an accept-reject step using the recomputed value of the truncated determinant $\mathcal{D}_{N_\lambda}(A)$. Strictly speaking [6] detailed balance only holds for the pure gauge step if links or sets of noninterfering links are updated in random order. For our QED2 runs we have found no statistically significant differences between the results obtained with ordered or random link updates. (A fully parallel code incorporating detailed balance will be used in all future truncated determinant simulations). The acceptance ratio for this procedure is tolerable (typically from 20-40%) because the typical fluctuation in $\log \mathcal{D}_{N_\lambda}(A)$ after a metropolis sweep is of order unity. (This is also the case in QCD4 with N_λ chosen large enough to include all the low energy chiral physics).
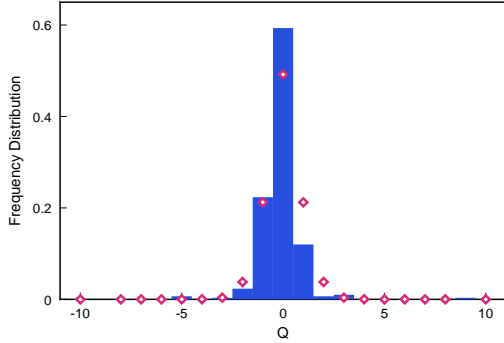
Some results obtained from truncated determi-

Figure 4. Q_{top} histogram in QCD4 for κ=0.1597 (diamonds- chiral result)

Figure 5. Static potential for quenched and dynamical QCD4. Error bars are largest for lightest mass and only shown for this case

nant simulations in QED2 are shown in Figs. 1-3. In Fig(1) the "pion" (i.e. pseudoscalar) correlators are shown for a very light quark: inclusion of the lowest 20 eigenvalues leads to correlators essentially identical to those in the fully unquenched theory. In Fig(2) the topological charge (Q_{top}) distribution is shown for the same parameters in quenched, unquenched and truncated determinant versions of the theory. The suppression of nonzero topological charge is basically complete when only 5% of the spectrum is included in the determinant. Fig.3 shows the onset of string breaking in the quark-antiquark potential measured from Wilson loops on a 16x16 lattice.

4. Truncated Determinant Simulations in QCD4

We have used the truncated determinant approach in QCD4 on a 12^3x24 lattice at β=5.9 for three kappa values, κ=0.1570, 0.1587 and 0.1597. Pion correlators were measured in order to perform a chiral extrapolation and determine the critical κ_c. 100 modes (up to $\simeq$370 MeV) were included in the quark determinant, with either one or two complete Metropolis pure gauge sweeps between determinant accept-reject steps (with acceptance varying betwen 20% and 50%). The topological charge can be extracted from an anomalous chiral identity, and is related to the trace of the inverse of $H = \gamma_5(\not{D} - m)$. This spectral sum converges rapidly: summing the lowest
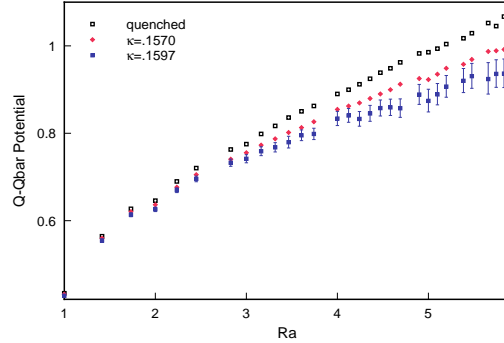
100 eigenvalues measures the topological charge (as per this definition) to a few percent. The histogram of measured topological charge in the lightest case, κ=0.1597 (corresponding to a pion mass of about 280 MeV) is shown in Fig.4, together with the analytic prediction for this distribution following from a chiral analysis [7].

In Fig.5 the static quark-antiquark potential (obtained from the correlation of Wilson lines in Coulomb gauge) shows a clear screening effect although true asymptotic flattening presumably occurs at distances where statistical fluctuations and finite volume effects dominate.

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